

Kristin Persson, Materials Project

FY 2014 Journal Publications:

PUBLISHED:

Primary:

- 1) "Resolving the True Band Gap of ZrNiSn Half-Heusler Thermoelectric Materials", J. Schmitt, Z. M. Gibbs, [G. J. Snyder](#), C. Felser, *Materials Horizons* in press, **2014**.
- 2) "*Nanograined half-Heusler semiconductors as advanced thermoelectrics: an ab-initio high-throughput statistical study*", J. Carrete, N. Mingo, S. Wang, and [S. Curtarolo](#), *Adv. Funct. Mater.* early view, **2014**. DOI: 10.1002/adfm.201401201.
- 3) "Thermoelectric performance of Tellurium-reduced quaternary p-type lead-chalcogenide composites", Sima Aminorroaya Yamini, H. Wang, Z. M. Gibbs, Y-Z. Pei, D. Mitchell, Shi Xue Dou, [G Jeffrey Snyder](#), *Acta Materialia* vol. 80, p. 365-372, **2014**. DOI:10.1016/j.actamat.2014.06.065
 - a. Acknowledgement: This work is supported by Australian Research Council (ARC) Discovery Early Career Award DE130100310, the Department of Education, Science and Technology (DEST) of Australia, the Materials Project funded by US Department of Energy's Basic Energy Sciences program under Grant No. EDCBEE, DOE contract DE-AC02-05CH11231 and the Air Force Office of Scientific Research—Multidisciplinary Research Program of the University Research Initiative (AFOSR-MURI) and the Russian Ministry of Education.
- 4) "*Optimization of Thermoelectric Efficiency in SnTe: The Case For the Light Band*", M. Zhou, Z. M. Gibbs, H. Wang, Y. Han, C. Xin, L. Li, [G. J. Snyder](#), *Physical Chemistry Chemical Physics* vol. 16, p. 20741-20748, **2014**. DOI: 10.1039/C4CP02091J.
- 5) "Lead-free halide perovskite solar cells with high photocurrents realised through vacancy modulation", M. H. Kumar, S. Dharani, T. Baikie, W. L. Leong, P. P. Boix, R. R. Prabhakar, T. Baikie, C. Shi, H. Ding, [R. Ramesh](#), [M. Asta](#), M. Graetzel, S. G. Mhaisalkar and N. Mathews, *Adv. Mater.* early view, **2014**. DOI: 10.1002/adma.201401991.
 - a. We acknowledge Rohit Abraham and Sudhanshu Shukla for assistance with fabrication and characterization. Sum Tze Chien and Alfred Huan are also acknowledged for scientific discussion. Financial support from NTU start-up grant M4081293, Singapore NRF through the Competitive Research Program (NRF-CRP4–2008–03) and the Singapore-Berkeley Research Initiative for Sustainable Energy (SinBeRISE) CREATE Programme is gratefully acknowledged. M.G. thanks the European Research Council for financial support under the Advanced Research Grant (ARG 247404) "Mesolight." Work at UC Berkeley was supported in part by the Materials Project program through the US Department of Energy, Basic Energy Sciences under grant No. EDCBEE, DOE Contract DE-AC02-05CH11231.

Collaborative:

- 6) "Low thermal conductivity of SnSe and existence of an easy axis for phonons", J. Carrete, N. Mingo, and [S. Curtarolo](#), *Appl. Phys. Lett.* vol. 105, p. 101907, **2014**. DOI: 10.1063/1.4895770

- 7) "New Light Harvesting Materials Using Accurate and Efficient Bandgap Calculations", I. E. Castelli, F. H\"user, M. Pandey, H. Li, Kristian S. Thygesen, B. Seger, A. Jain, [K. Persson](#), [G. Ceder](#), and Karsten W. Jacobsen, *Adv. Energy Mater.* pre-print, **2014**.
DOI:10.1002/aenm.201400915 (2014)
- 8) "Elastic Properties of Chemical-Vapor-Deposited Monolayer MoS₂, WS₂, and Their Bilayer Heterostructures", K. Liu, Q. Yan, M. Chen, W. Fan, Y. Sun, J. Suh, D. Fu, S. Lee, J. Zhou, S. Tongay, J. Ji, [J. B. Neaton](#), and J. Wu, *Nano Lett.* vol. 14(9), p. 5097, **2014**. DOI: 10.1021/nl501793a
- 9) "A Proposed Definition of Crystal Substructure and Substructural Similarity," L. Yang, S. Dacek, [G. Ceder](#), *Phys. Rev. B* vol. 90, p. 054102, **2014**. DOI: 10.1103/PhysRevB.90.054102.
- 10) "Origin of High Electrolyte-Electrode Interfacial Resistances in Lithium Cells Containing Garnet Type Solid Electrolytes", L. Cheng, E. J. Crumlin, W. Chen, R. Qiao, H. Hou, S. F. Lux, V. Zorba, R. Russo, R. Kostecki, Z. Liu, [K. Persson](#), W. Yang, J. Cabana, T. Richardson, G. Chen, and M. Doeff, *Phys Chem Chem Phys*, vol. 16, p. 18294-18300, **2014**.
DOI: 10.1039/C4CP02921F.
- 11) "A RESTful API for exchanging Materials Data in the AFLOWLIB.org consortium", R. H. Taylor, F. Rose, C. Toher, O. Levy, K. Yang, M. Buongiorno Nardelli, and [S. Curtarolo](#), *Comp. Mat. Sci.* vol. 93, p. 178-193, **2014**. DOI: 10.1016/j.commatsci.2014.05.014.
- 12) "Analysis of Charged State Stability for Monoclinic LiMnBO₃ Cathode", J.C. Kim, X. Li, C.J. Moore, S-H Bo, P.G. Khalifah, C.P. Grey, [G. Ceder](#), *Chem. Mater.* vol. 26(14), p. 4200-4206, **2014**. DOI: 10.1021/cm5014174.
- 13) "Distinct Solid-Electrolyte-Interphases on Sn (100) and (001) Electrodes Studied by Soft X-Ray Spectroscopy", Qiao, R., Lucas, I. T., Karim, A., Syzdek, J., Liu, X., Chen, W., [Persson, K.](#), Kostecki, R., Yang, W., *Adv. Mater. Interfaces*, vol. 1(3), p. 1300115, **2014**.
DOI: 10.1002/admi.201300115.
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- 14) "Nanoscale Stabilization of Sodium Oxides: Implications for Na-O₂ Batteries", S.Y. Kang, Y. Mo, [S.P. Ong](#), [G. Ceder](#), *Nano Letters* vol. 14, p. 1016-1020, **2014**.
DOI:10.1021/nl404557w.
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